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First-principles simulation of magnetic defects on the substrate of noisy superconducting qubits[1] NICOLE ADELSTEIN, JONATHAN DUBOIS, VINCENZO LORDI, Lawrence Livermore National Laboratory — Superconducting qubits represent one of the more promising routes to realization of a scalable quantum computer. Current performance as measured by the lifetime of quantum states in these systems is, however, largely limited by an as yet unidentified source of low frequency flux noise. Recent experimental and theory efforts suggest that the noise in flux qubits arises from hopping of unpaired spins on the silica or sapphire substrate. In addition, noise could be due to defects with low energy magnetic excited states, though neither noise source is known at the atomic level. We have performed a comprehensive study of the magnetic defects on the surface of SiO_2 and investigated barriers to magnetic fluctuations using first-principles density functional theory. Within this framework, we show how defects, such as oxygen vacancies, and adsorbents, such as water, on the substrate represent possible sources of magnetic flux fluctuations.

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